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ADVANCED REACTOR SAFEGUARDS

Using Machine Learning to Improve Efficiency and Accuracy of Burnup Measurements at PBR Reactors

PRESENTED BY

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Motivations of the Work

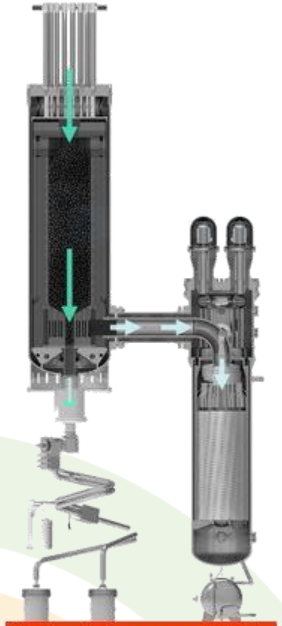
- Burnup measurement is the key to deciding if the pebble should be discharged or recycled during the operation of a PBR reactor
- Burnup measurement faces two challenges:
  - High throughput
  - High accuracy
- Objectives
  - Create and validate a workflow for modeling and simulation of both burnup and gamma-ray detection
  - Build ML models
  - Study performance of ML models

FY23 Technical Tasks

- Modeling and simulation
  - Add collimator to the workflow to reduce the flux
  - Validation of the simulation workflow
    - Develop full PBMR model
    - Automate result generation
    - *Validate the burnup results*
    - *Validate the conversion of Serpent output*
- Explore the explainability of the ML model

Validation of Burnup Model

Modeling and Simulation Workflow

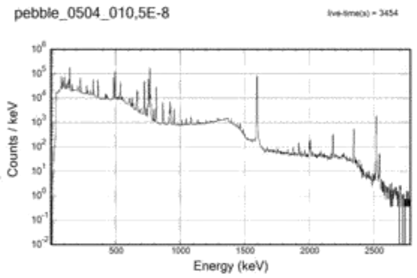


SERPENT SIMULATION

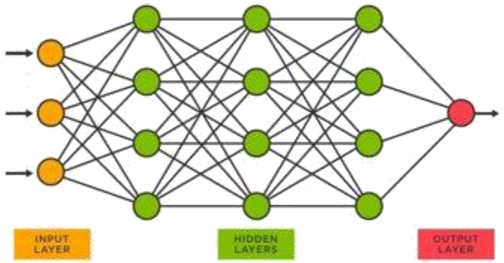
Include burnup model and collimation

GAMMA SOURCE

GADRAS SOFTWARE



GAMMA SPECTRA



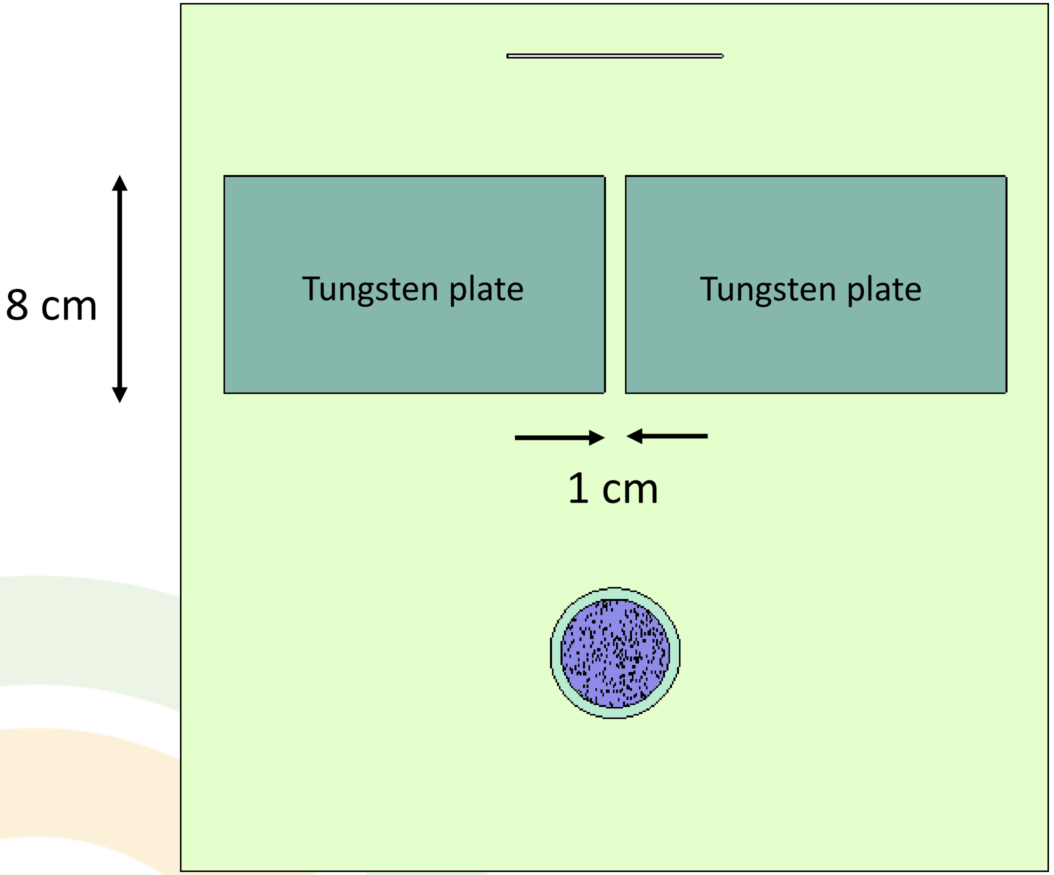
ML ALGORITHM

PREDICTION

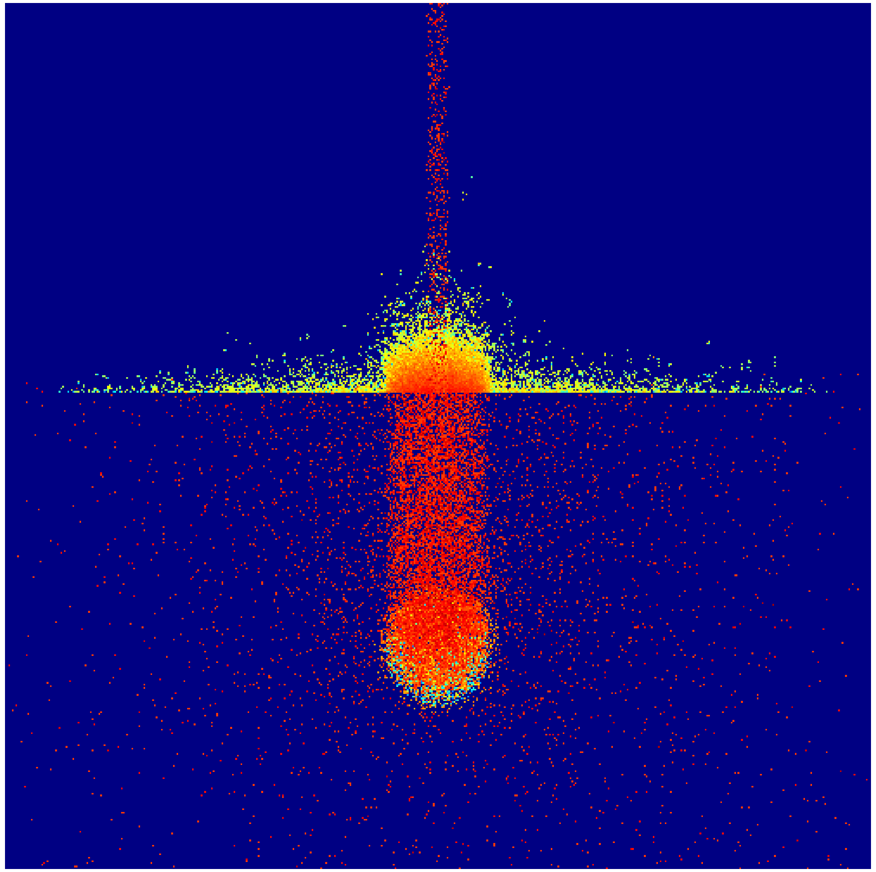
Collimation Analysis

- Ejected pebbles from the core are highly radioactive, so collimator is needed to reduce the flux seen by the detector.
- A few options (MCNP, Geant4, Serpent) were considered based on ease of implementation, efficiency of simulation and accuracy.
- We decided to model the collimator directly into the source model in Serpent, eliminating the need to validate data translation to/from an external code.

Collimation Analysis (Cont'd)

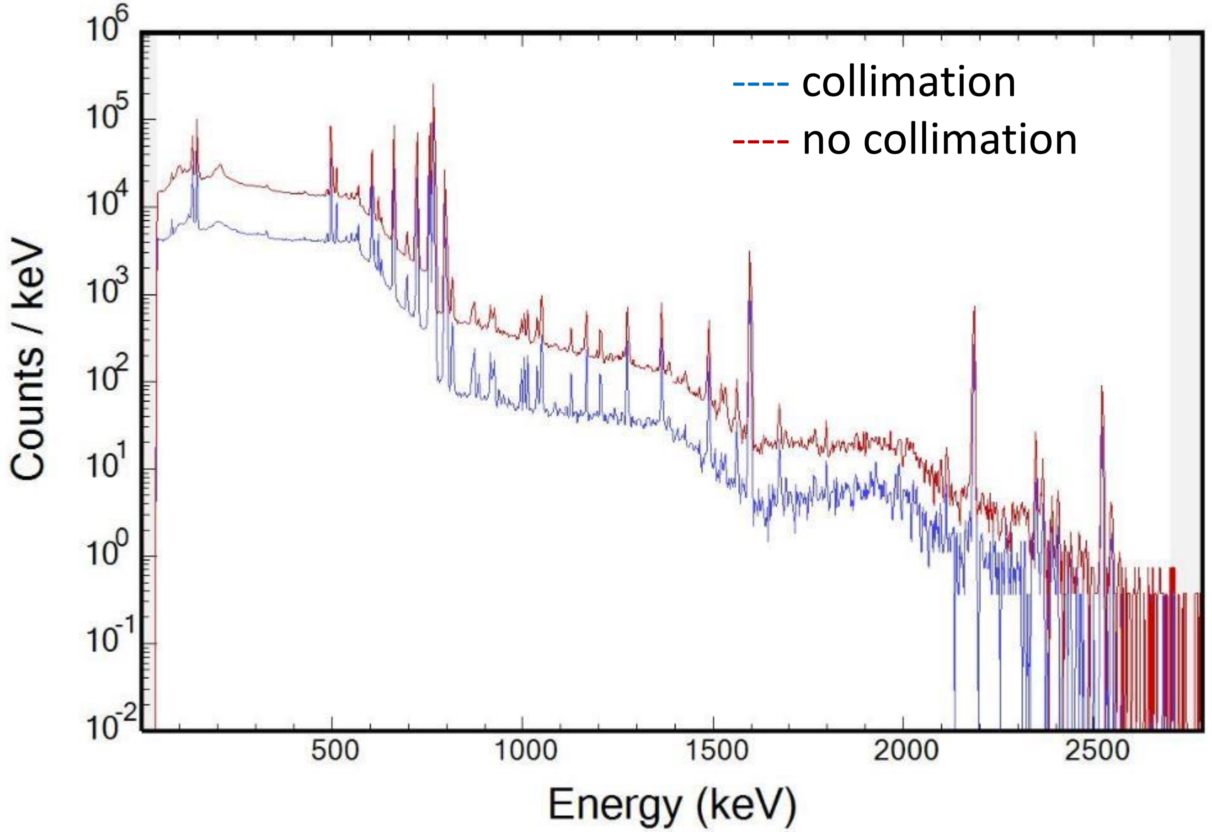


Source detector geometry including collimator

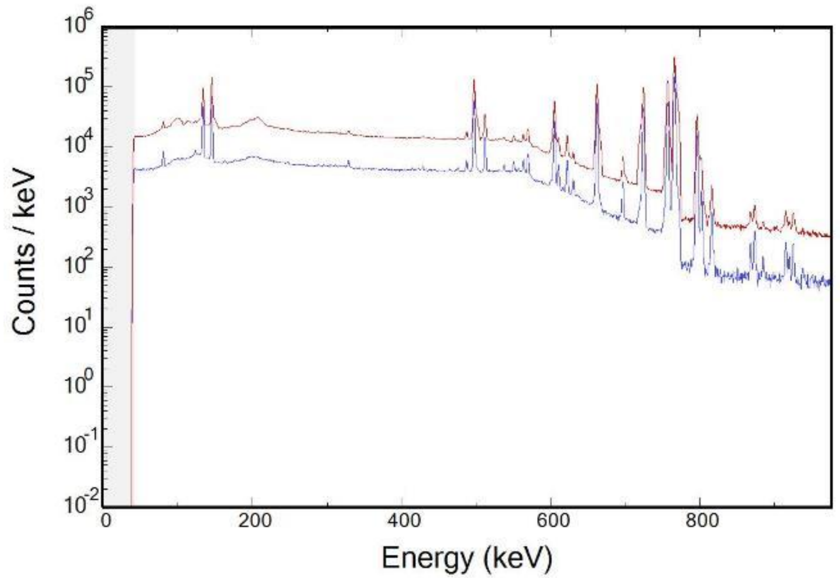


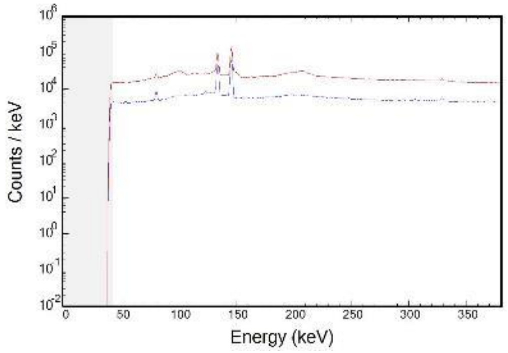
Photon tracks showing collimator effects

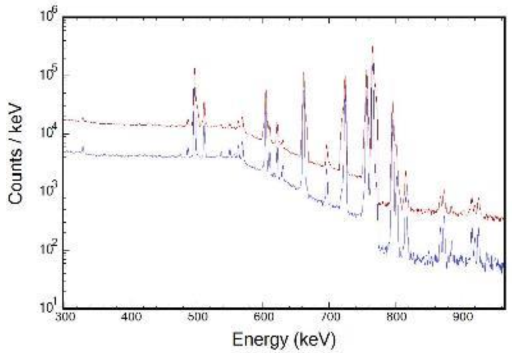
Collimation Analysis (Cont'd)



Full spectra with and without collimation



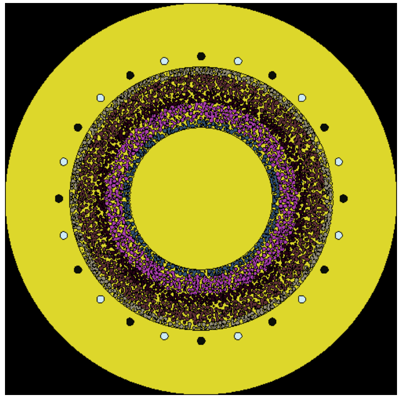




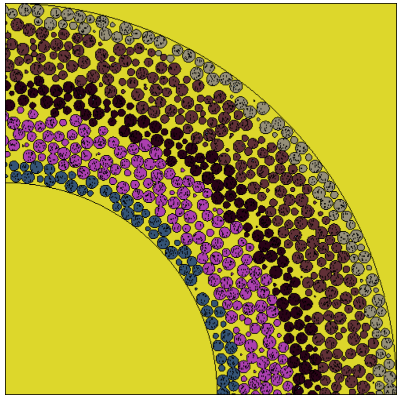
Collimation effect on specific energy ranges

Full Core Model for Burnup Validation

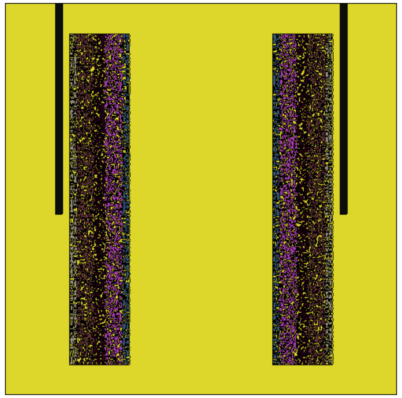
- Compared to the lattice model, a full-core model allows
  - More realistic flux and power distribution, hence resulting in more accurate burnup on a pebble per its location.
  - Full core modeling generates a potential to describe the effects of pebble flow path on the overall burnup
  - More accurate simulation to validate or compare to experimental data
  - The effect of control and burnup poisons are better described in a full core model



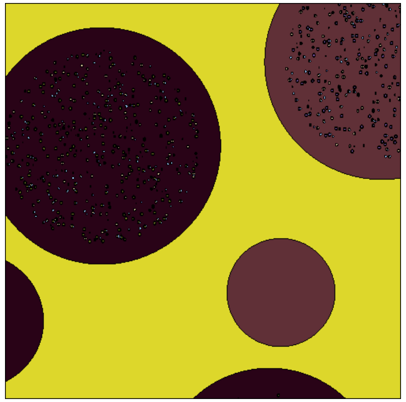
Top view



Zoomed In Quarter Core



Cut through Side View



Pebble in Core

Full core model of a PBMR design

Benefits of Using Serpent In Simulation

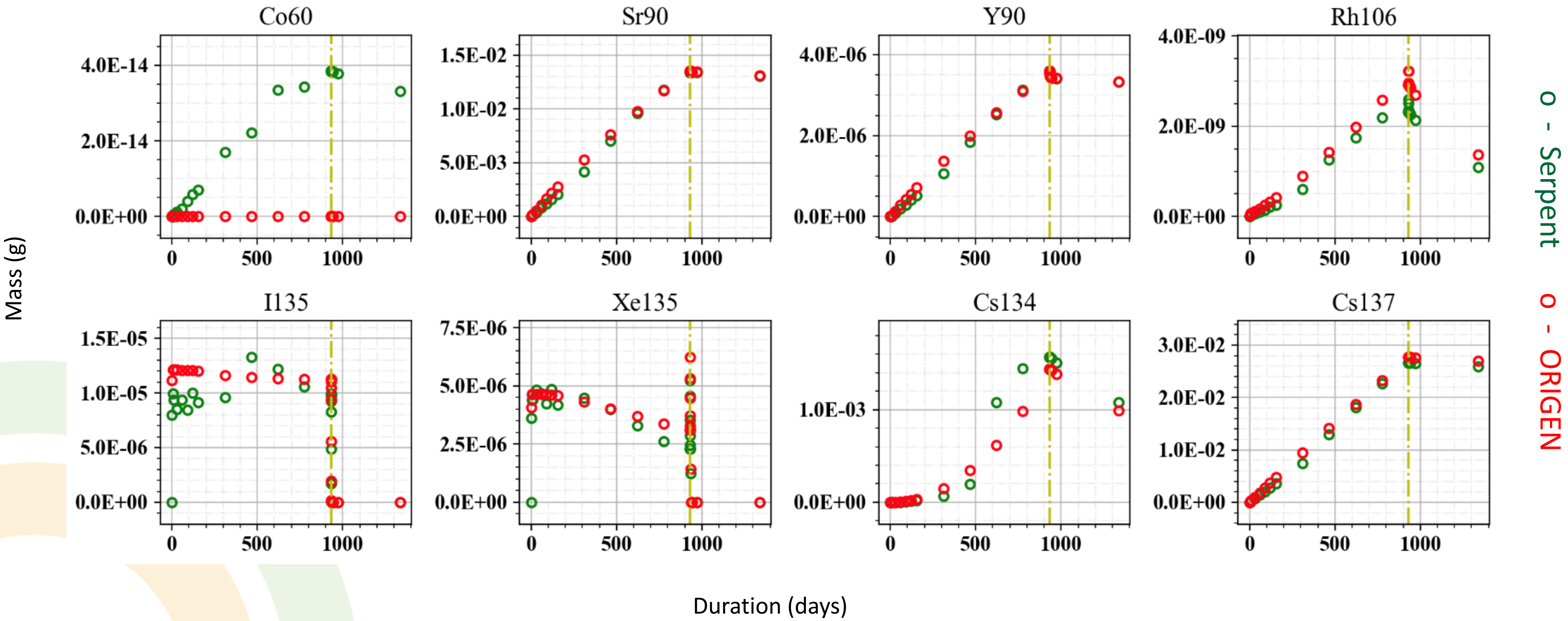
- Serpent models are defined to represent the realism of the intended geometry.
  - Explicit particle location definitions.
- Sensitivity study can be implemented without having to go through the hassle of generating zonal group cross-sections.
- You have the option of switching on and off the reproducibility on a specific simulation.
- A variety of detector and visualization options.
- Facilitates easy implementation of automation for simulation processes.

Simulation Results

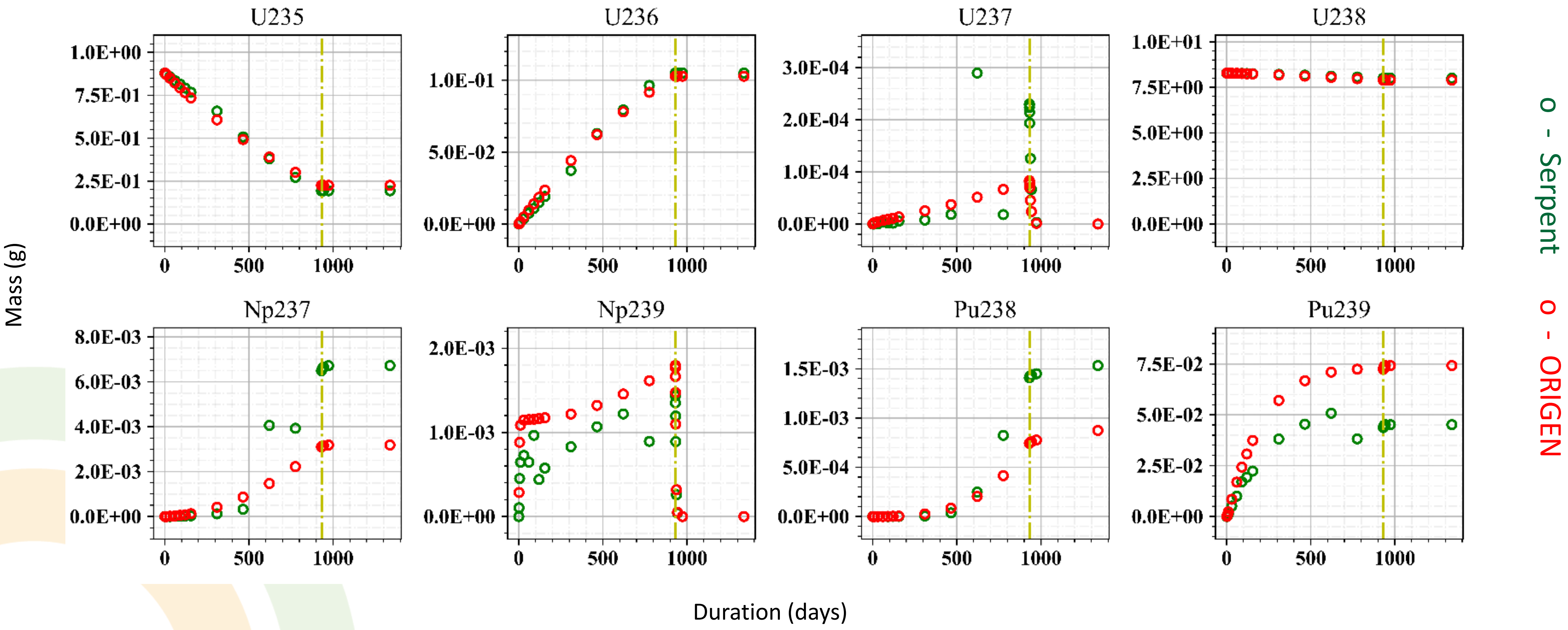
Pebble	Volume (cm3)	Burnup (MWD/kgU)	Initial density of U (g/cm3)	Initial mass of U (gU)	Initial mass of U (kgU)	Duration of Burnup (days)	Power (MW)	Specific power (MW/KgU)
1	9.8E-01	6.98E+01	9.20	9.00	9.00E-03	4.66E+02	1.35E-03	1.50E-01
2	9.8E-01	6.20E+01	9.20	9.00	9.00E-03	4.66E+02	1.18E-03	1.33E-01
3	9.8E-01	5.15E+01	9.20	9.00	9.00E-03	4.66E+02	9.76E-04	1.10E-01
4	9.8E-01	3.86E+01	9.20	9.00	9.00E-03	4.66E+02	7.32E-04	8.29E-02
5	9.8E-01	3.33E+01	9.20	9.00	9.00E-03	4.66E+02	6.31E-04	7.14E-02

Average burnup over 5 pebbles: ~108 MW/MTU

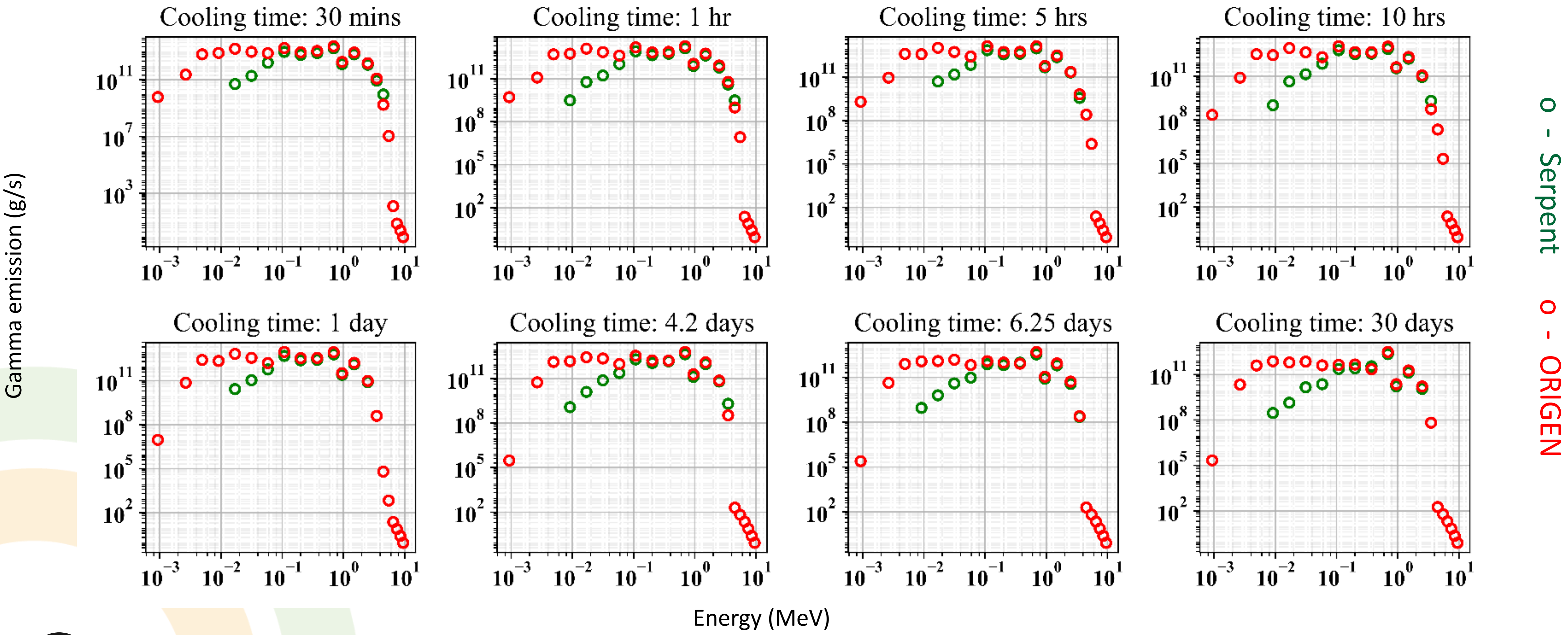
Simulation Results – (isotope verification)



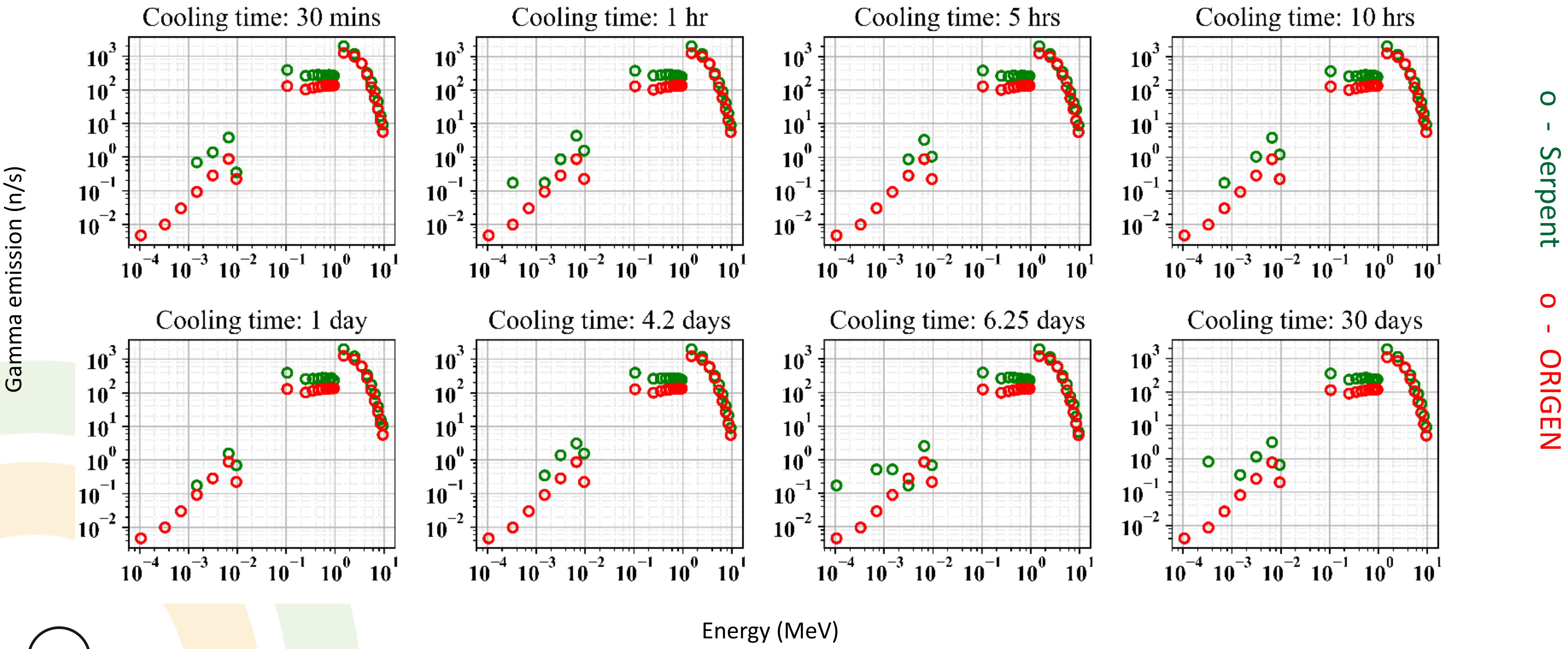
Simulation Results – (isotope verification)



Simulation Results – (emission verification)



Simulation Results – (emission verification)



Explainability of ML Model

Machine Learning for Burnup Measurement

- We have demonstrated promising results with our ML models
  - Significantly outperforming linear regression method
  - Specifically, high performance at short cooling
- Results accepted for publication

C. X. Soto et al. "A Better Method to Calculate Fuel Burnup in Pebble Bed Reactors Using Machine Learning," *Nuclear Technology*, DOI 10.1080/00295450.2023.2200573

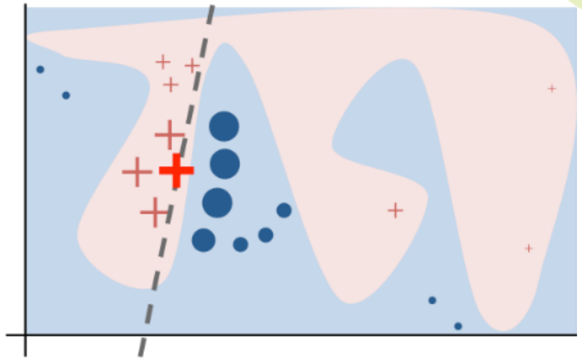
- However, Neural Network-based **ML models are inherently opaque**
  - Learned feature representations are not easily interpretable
  - Therefore, confidence and downstream impact of this work may be limited in its present state
  - Also, short-cooling performance merits deeper investigation

Approaches to ML Explainability/Interpretation

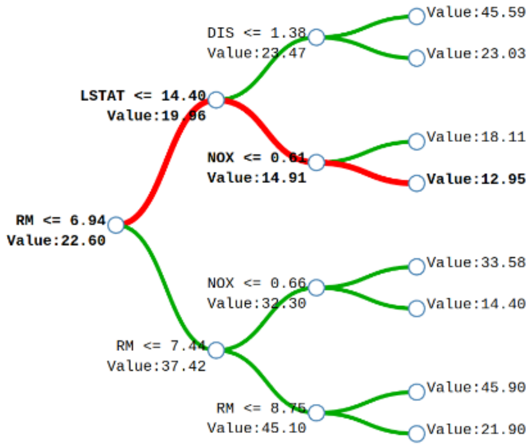
- Two classes of approaches to explain neural networks
  - *Interpretation* seeks to understand the mechanistic operation of a neural network model
    - Identifying meaning for model weights; very challenging
  - *Explainability* seeks to identify the causal links between an input data and a result, irrespective of the ML model type
    - Identifying the features that corresponded to a particular model prediction
- We chose a feature-based explainability approach and identified two types of surrogate models/tools
  - **LIME**: Linear Interpretable Model-agnostic Explanations
  - **SHAP**: SHapley Additive exPlanations

Explainability Study

- LIME and SHAP operate differently and complement one another
  - LIME produces **linear models** generated by dense feature perturbation
  - SHAP produces **tree ensembles** based on game-theoretic feature contribution
  - *Feature density poses a problem for both, though*
- We take a tiered approach:
  - Iteratively re-bin spectra to perform LIME feature selection
  - Filter, re-bin, and re-select until at raw spectral resolution
  - Use final energy bins as SHAP input features for comparison



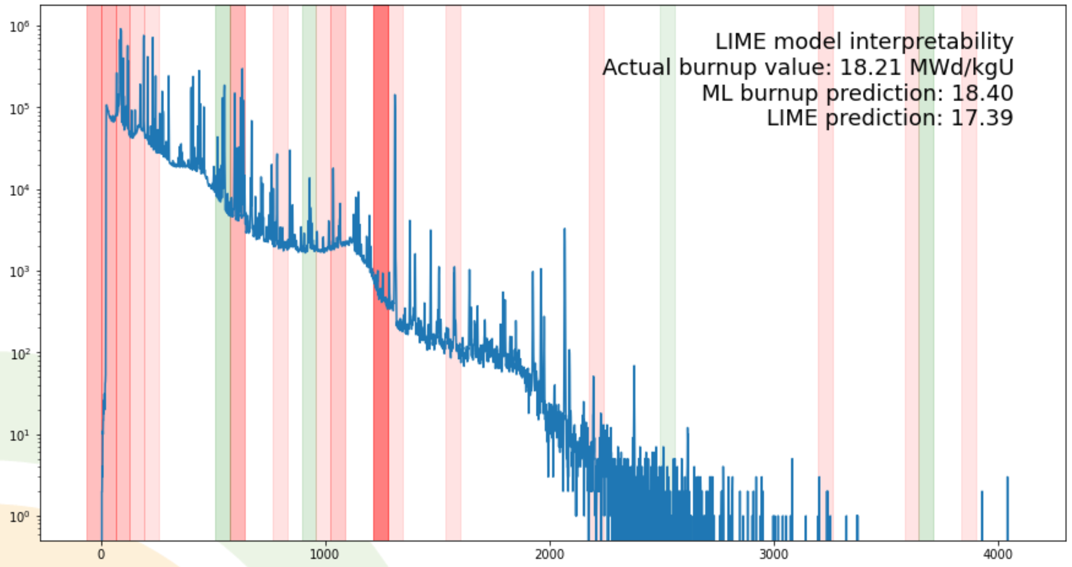
LIME works by creating linear decision boundaries using perturbed feature values

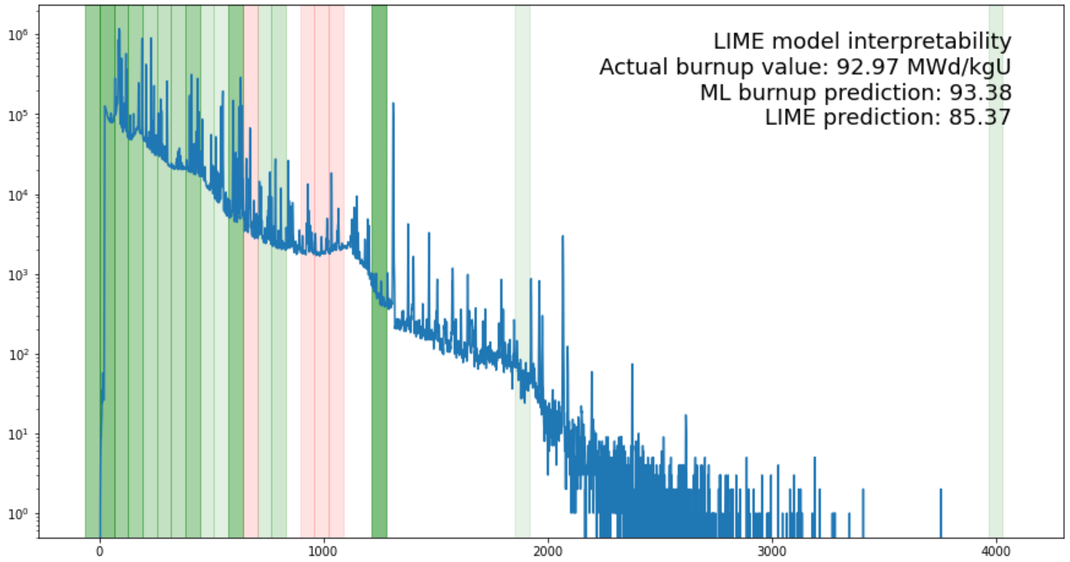


SHAP works by creating an ensemble of tree models based on Shapley-value estimations for feature contributions

Results and Ongoing Work

- Initial results (*figures below*) highlight low-resolution spectral energy bands with likely causal relationships to burnup





Next Steps

- Modeling and simulation
  - Produce simulation data of full-core simulation and compare with ORNL work and published data on PMBR400
  - Presentation at the INMM Meeting
  - Finalize the integration of collimation simulation in the workflow
- Explainability
  - We are now assessing across cooling and acquisition time datasets, and investigating feature consistency
  - Next step is to iterate down to spectral resolution across burnup, cooling and acquisition conditions

Acknowledgement

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- Thanks for Drs. Jianwei Hu and Donny Hartanto from ORNL for discussions on modeling and simulation of PBMR400 reactor.

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